

# Analytical Structure Matching and Very Precise Approach to the Coulombic Quantum Three-Body Problem

TAN, Shi-Na \*

Institute of Theoretical Physics, CAS, P.O.Box 2735, Beijing 100080, P.R.China

## Abstract

A powerful approach to solve the Coulombic quantum three-body problem is proposed. The approach is exponentially convergent and more efficient than the Hyperspherical Coordinate(HC) method and the Correlation Function Hyperspherical Harmonic(CFHH) method. This approach is numerically competitive with the variational methods, such as that using the Hylleraas-type basis functions. Numerical comparisons are made to demonstrate them, by calculating the non-relativistic & infinite-nuclear-mass limit of the ground state energy of the helium atom. The exponentially convergency of this approach is due to the full matching between the analytical structure of the basis functions that I use and the true wave function. This full matching was not reached by almost any other methods. For example, the variational method using the Hylleraas-type basis does not reflect the logarithmic singularity of the true wave function at the origin as predicted by Bartlett and Fock. Two important approaches are proposed in this work to reach this full matching: the coordinate transformation method and the asymptotic series method. Besides these, this work makes use of the least square method to substitute complicated numerical integrations in solving the Schrödinger equation, without much loss of accuracy; this method is routinely used by people to fit a theoretical curve with discrete experimental data, but I use it here to simplify the computation.

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## 1 INTRODUCTION

Most approximate methods to solve a linear partial differential equation, such as the stationary state Schrödinger equation, are actually to choose an  $N$ -dimensional subspace of the infinite-dimensional Hilbert space and then to reduce the partial differential equation to  $N$  linear algebraic equations defined in this subspace. The efficiency of this kind of methods is mainly determined by whether one

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\*E-mail: tansn@itp.ac.cn

can use sufficient small  $N$  to reach sufficient high accuracy, i.e., make the vector most close to the true solution in this subspace sufficiently close to the true solution while keeping the dimension  $N$  not too large to handle.

Most methods to solve the Coulombic quantum three-body problem belong to this class, except for some variational methods that make use of some non-linear variational parameters. The differences between different methods of this kind mainly lie in different choices of the subspaces of the Hilbert space, i.e., different choices of the basis functions to expand the wave function.

Theoretically, any discrete and complete set of basis functions may be used to expand the wave function, and the convergency is easy to fulfilled. But actually, the convergency is often slow and makes sufficient accuracy difficult to achieve. The naive hyperspherical harmonic function method[1-3] in solving the Coulombic quantum three-body problem is such an example—this slow convergency can be illustrated by an analogous and simple example: to expand the function  $f(x) = \sqrt{1-x^2}$  ( $-1 \leq x \leq +1$ ) as a series of the Legendre polynomials of  $x$ . This series is convergent like  $N^{-s}$ , where  $s$  is a positive constant not large and  $N$  is the number of Legendre polynomials involved. The reason for this slow convergency is that  $f(x)$  is singular at  $x = \pm 1$  but the Legendre polynomials of  $x$  are not. I call this the mismatching between the analytical structures of the basis functions (the polynomials of  $x$ ) and  $f(x)$ .

The correlation function hyperspherical harmonic(CFHH) method[4] were proposed to overcome this difficulty. The spirit of this method can be simply illustrated, still using the above example: to divide  $f(x)$  by an appropriately selected function(called the correlation function) to cancel the low order singularities of  $f(x)$  at  $x = \pm 1$ , then to expand the remaining function by the Legendre polynomials of  $x$ . This time, the series is still convergent as  $N^{-s}$ , but  $s$  is increased by an amount depending on how many orders' singularities have been canceled.

From this simple discussion one can see that the singularities of the function  $f(x)$  are not completely canceled by the correlation function, although more sophisticated correlation function can cancel more orders' singularities.

A very simple approach to *totally* eliminate the singularity is to make an appropriate coordinate transformation, and in the same time thoroughly give up the original hyperspherical harmonic function method, not just repair it. For example, for  $f(x) = \sqrt{1-x^2}$ , one may write  $x = \sin \theta$ , where  $-\pi/2 \leq \theta \leq \pi/2$ , then  $f(x) = \cos \theta$  and one can expand  $f(x)$  as the series about the Legendre polynomials of  $(2/\pi)\theta$ . This time the series is *factorially* convergent. The reason is that the analytical structures of  $f(x)$  and  $P_l((2/\pi)\theta)$  match—they are both analytical functions on the whole complex plane of  $\theta$ .

Another useful approach to solve this problem is to use the asymptotic series. Still considering the

example  $f(x) = \sqrt{1-x^2}$ , one may write the Taylor series

$$f(x) = f_0 + f_1x + f_2x^2 + f_3x^3 + \cdots .$$

Of course, this series is slowly convergent near  $x = \pm 1$ . But one can use the following asymptotic series to calculate  $f_n$  when  $n$  is large:

$$f_n = ((-1)^n + 1)(c_{3/2}n^{-3/2} + c_{5/2}n^{-5/2} + c_{7/2}n^{-7/2} + \cdots) ,$$

or, equivalently,

$$f_n = ((-1)^n + 1) \sum_{s=1/2}^{1/2+L} \tilde{f}_s \frac{s!}{n!(s-n)!} ,$$

where  $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots, \frac{1}{2} + L$ , and  $s! \equiv \Gamma(s+1)$ . For a given  $n \gg 1$ , the error of this formula is minimized when  $L/n \simeq 2/3$ , and the minimum error is about  $\sqrt{\frac{27}{2\pi^2}} n^{-2} 3^{-n}$ , which exponentially decreases with  $n$  increasing. Using such kind of asymptotic formulae to calculate the high order coefficients of the Taylor series, one can expand the singular function  $f(x)$  at high precision, with only finite linear parameters,  $f_0, \dots, f_n$  and  $\tilde{f}_{1/2}, \dots, \tilde{f}_{1/2+L}$ .

Now I introduce an alternative approach to reduce a differential equation to a given finite dimensional subspace  $\mathcal{L}_N$  of the Hilbert space. Here  $N$  is the dimension of the subspace. The central problem is how to reduce an operator  $O$  in the Hilbert space, e.g., the kinetic energy operator or the potential energy operator, to an  $N \times N$  matrix in the given subspace. For a state  $\Psi \in \mathcal{L}_N$ , the state  $\Psi_O \equiv O\Psi$  usually  $\notin \mathcal{L}_N$ . To reduce  $O$  into an  $N \times N$  matrix means to find a state  $\Xi \in \mathcal{L}_N$  to approximate  $\Psi_O$ . The usual approach to select  $\Xi$  is to minimize

$$(\Xi - \Psi_O, \Xi - \Psi_O) ,$$

where  $(,)$  is the innerproduct of the Hilbert space. This approach will reduce  $O$  to a matrix with elements

$$O_{ij} = (\phi_i, O\phi_j) ,$$

where  $\phi_i \in \mathcal{L}_N$  is a set of orthonormal basis in  $\mathcal{L}_N$ , satisfying  $(\phi_i, \phi_j) = \delta_{ij}$ ,  $1 \leq i, j \leq N$ . In numerical calculation, the innerproduct is usually computed by numerical integration, which needs sufficient accuracy and might be complicated. An alternative approach that does not need these integrations is to write the states as wavefunctions under a particular representation(e.g., the space-coordinate representation), and then select  $\Xi$  to minimize

$$\sum_a |\Xi(x_a) - \Psi_O(x_a)|^2 ,$$

where  $x_a$  is some sample points in the defining area of the wavefunctions. In order to ensure  $\Xi$  to be a good approximation of  $\Psi_O$ , the sample points should be appropriately chosen. Usually the number of the sample points is greater than and approximately proportional to  $N$ , and the separation between

two neighboring sample points should be less than the least quasi-semiwavelength of a wavefunction in  $\mathcal{L}_{\mathcal{N}}$ .

This alternative approach (I call it the least square method) leads to a reduction of the operator  $O$ :

$$\tilde{O}_{ij} = (\tilde{\phi}_i, O\tilde{\phi}_j)' ,$$

where  $(, )'$  is a pseudo-innerproduct defined as  $(\phi, \psi)' \equiv \sum_a \phi^*(x_a)\psi(x_a)$  for arbitrary  $\phi$  and  $\psi$ , and  $\tilde{\phi}_i$  is a set of pseudo-orthonormal basis in  $\mathcal{L}_{\mathcal{N}}$  satisfying  $(\tilde{\phi}_i, \tilde{\phi}_j)' = \delta_{ij}$ . We find that this approach is very similar to the usual one, except that a discrete sum over sample points takes the place of the usual innerproduct integration. And there is a great degree of freedom in the selection of the sample points. In fact, as soon as the sample points are selected according to the spirit mentioned above, the accuracy of the solution of the differential equation usually will not decrease significantly. The major factor that determines the accuracy of the solution is the choice of the subspace  $\mathcal{L}_{\mathcal{N}}$ , which has been discussed to some extent in previous pages.

In this work, solving the simplest quantum three-body problem, the three methods discussed above are all used: the coordinate transformation method, the asymptotic series method, and the least square method. A high precision is reached for the ground state energy of the ideal helium atom, and the solution has also some merit in comparison with the Hyleraas-type variational solution[5,6]. In section 2 the Bartlett-Fock expansion[7,8,9] is studied, in order to reflect the analytical structure of the wavefunction near the origin. In this study, the asymptotic series are used to represent the hyper-angular dependence of the wavefunction. In section 3 the  $(u, w)$  coordinate system is used to study the hyper-angular dependence of the wavefunction. This coordinate system cancels the singularity of the hyper-angular functions totally. The relationship between this coordinate system and the Hyleraas-type variational method is also discussed. The least square method is used to reduce the hyper-angular parts of the kinetic energy operator and the potential energy operator to finite-dimensional matrices. In section 4 the connection of the outer region solution and the inner region Bartlett-Fock expansion is studied, using the least square method. In section 5 the numerical result is presented and compared with those of other methods. Some explanations are made. In section 6 some discussions are presented and some future developments are pointed out.

## 2 BARTLETT-FOCK EXPANSION

Considering an S state of an ideal helium atom, that is, assuming an infinite massive nucleus and infinite light speed, one may write the Schrödinger equation

$$-2t(\partial_x^2 + \partial_y^2 + \partial_z^2 + \frac{1}{z}\partial_z)\psi + V\psi = E\psi , \quad (1)$$

where  $x = r_1^2 - r_2^2$ ,  $y = 2r_1r_2 \cos \theta_{12}$ ,  $z = 2r_1r_2 \sin \theta_{12}$ , and  $t = r_1^2 + r_2^2 = \sqrt{x^2 + y^2 + z^2}$ .  $r_1$  and  $r_2$  are the distances of the electrons from the nucleus, and  $\theta_{12}$  is the angle formed by the two electronic position vectors measured from the nucleus. In this equation, an S state is assumed, so the wavefunction  $\psi$  is only dependent on  $r_1$ ,  $r_2$  and  $\theta_{12}$ , or, equivalently,  $x$ ,  $y$ , and  $z$ . The atomic unit, i.e.,  $\hbar = m_e = e^2/(4\pi\epsilon_0) = 1$ , is assumed throughout this paper. The potential energy is

$$V = -\frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \quad (2)$$

where  $r_{12}$  is the distance between the two electrons.

$$r_1 = \sqrt{\frac{t+x}{2}}, \quad r_2 = \sqrt{\frac{t-x}{2}}, \quad r_{12} = \sqrt{t-y}. \quad (3)$$

The Bartlett-Fock expansion is

$$\psi = \sum_{n,k} \psi_{n,k} t^n \frac{(\ln t)^k}{k!}, \quad (4)$$

where  $n = 0, 1/2, 1, 3/2, 2, \dots$ , and  $k = 0, 1, 2, \dots$ .  $\psi_{n,k}$  only depends on the two hyper-angles, say,  $\alpha \equiv x/t$  and  $\beta \equiv y/t$ , and does not depend on the hyper-radius,  $\rho \equiv \sqrt{t}$ . When  $k > n$ ,  $\psi_{n,k} \equiv 0$ .

Using the coordinates  $t$ ,  $\alpha$ , and  $\beta$ , one may rewrite the Schrödinger equation (1) as

$$(\partial_t^2 + \frac{3}{t}\partial_t + \frac{1}{t^2}L_0)\psi = (vt^{-3/2} + pt^{-1})\psi, \quad (5)$$

where  $p \equiv -E/2$ , and

$$L_0 = (1 - \alpha^2)\partial_\alpha^2 - 2\alpha\beta\partial_\alpha\partial_\beta + (1 - \beta^2)\partial_\beta^2 - 3\alpha\partial_\alpha - 3\beta\partial_\beta; \quad (6)$$

$$v = -\frac{\sqrt{2}}{\sqrt{1+\alpha}} - \frac{\sqrt{2}}{\sqrt{1-\alpha}} + \frac{1/2}{\sqrt{1-\beta}}. \quad (7)$$

Substituting eq.(4) into eq.(5), and comparing the corresponding coefficients before  $t^n(\ln t)^k$ , one will obtain

$$L_n\psi_{n,k} + (2n+2)\psi_{n,k+1} + \psi_{n,k+2} = v\psi_{n-\frac{1}{2},k} + p\psi_{n-1,k}, \quad (8)$$

where  $L_n \equiv n(n+2) + L_0$ .

The functions  $\psi_{n,k}$  are solved out in the order with  $n$  increasing; and for each  $n$ , with  $k$  decreasing. The physical area of  $(\alpha, \beta)$  is the unit circle:  $\alpha^2 + \beta^2 \leq 1$ . And the function  $\psi_{n,k}(\alpha, \beta)$  may have singularities at  $\alpha = \pm 1$  and at  $\beta = 1$ . The singularities are of these kinds:  $(1 - \alpha)^s$ ,  $(1 + \alpha)^s$ , and  $(1 - \beta)^s$ , with  $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$ . So one may write the Taylor series in the  $(\alpha, \beta)$  unit circle:

$$\psi_{n,k}(\alpha, \beta) = \sum_{a,b=0}^{\infty} \psi_{n,k,a,b} \alpha^a \beta^b. \quad (9)$$

The singularities make the usual cutoff,  $a + b \leq L_f + L_s$ , inappropriate, because the error decreases slowly when  $L_f + L_s$  increases. But since we have known the forms of the singularities, we can

write the asymptotic formulae to calculate those high order Taylor coefficients that have important contributions:

$$\psi_{n,k,a,b} = \sum_{s=\frac{1}{2}}^{L_i-\frac{1}{2}} \tilde{\psi}_{n,k,b,s} \binom{s}{a} [1 + (-1)^a] ; \quad (10-1)$$

$$\psi_{n,k,a,b} = \sum_{s=\frac{1}{2}}^{L_i-\frac{1}{2}} \tilde{\psi}_{n,k,a,s} \binom{s}{b} (-1)^b . \quad (10-2)$$

Eq.(10-1) is appropriate when  $a \gg b$  and  $a \gg 1$ , while eq.(10-2) is appropriate when  $b \gg a$  and  $b \gg 1$ .  $\binom{s}{a} \equiv (s!)/[a!(s-a)!]$ , and  $s! \equiv \Gamma(s+1)$ . Here I have assumed the state is a spin-singlet, and thus  $\psi_{n,k}(-\alpha, \beta) = \psi_{n,k}(\alpha, \beta)$ . For a spin-triplet, the factor  $[1 + (-1)^a]$  in eq.(10-1) should be substituted by  $[1 - (-1)^a]$ .

In my actual calculation, the  $(a, b)$  plane is divided into four areas:

the finite area:  $0 \leq a, b \leq L_f$  and  $a + b \leq L_f + L_s$  ( $L_f \gg L_s \gg 1$ ),

the  $a$ -asymptotic area:  $a > L_f$  and  $b \leq L_s$ ,

the  $b$ -asymptotic area:  $b > L_f$  and  $a \leq L_s$ ,

and the cutoff area: the remain area.

Eq.(10-1) is used in the  $a$ -asymptotic area, and eq.(10-2) is used in the  $b$ -asymptotic area, while the contribution from the cutoff area is neglected for it is extremely tiny when  $L_f \gg L_s \gg 1$ .

In a word, a relevant hyper-angular function is described by a finite set of parameters up to a high precision. These parameters are some Taylor coefficients and some asymptotic coefficients. To operate with some functions of this kind means to operate with the corresponding sets of parameters. The relevant operations are: addition of two functions—adding the corresponding parameters of the two sets; multiplying a function by a constant—multiplying each parameter in the set by the constant; multiplying a function by  $v(\alpha, \beta)$ (eq.(7))—an appropriate linear transformation of the set of parameters of the multiplied function; solving an equation  $L_n f = g$  with  $g$  known and  $f$  unknown—solving a set of linear equations about the parameters corresponding to  $f$ . Here, I write the relevant linear equations corresponding to the equation  $L_n f = g$ :

$$[n(n+2) - (a+b)(a+b+2)]f_{a,b} + (a+1)(a+2)f_{a+2,b} + (b+1)(b+2)f_{a,b+2} = g_{a,b} ; \quad (11-0)$$

$$[n(n+2) - (b+s)(b+s+2)]\tilde{f}_{b,s} + (s+1)(2s+2b+3)\tilde{f}_{b,s+1} + (b+1)(b+2)\tilde{f}_{b+2,s} = \tilde{g}_{b,s} ; \quad (11-1)$$

$$[n(n+2) - (a+s)(a+s+2)]\tilde{f}_{a,s} + (s+1)(2a+2s+3)\tilde{f}_{a,s+1} + (a+1)(a+2)\tilde{f}_{a+2,s} = \tilde{g}_{a,s} . \quad (11-2)$$

The detailed order to solve  $\psi_{n,k}$  is:

Case 1:  $n = [n] + \frac{1}{2}$ , where  $[n]$  is an integer. In this case, solve  $\psi_{n,[n]}$  from eq.(8 <sub>$n,[n]$</sub> ); and then solve  $\psi_{n,[n]-1}$  from eq.(8 <sub>$n,[n]-1$</sub> );  $\cdots$ ; at last solve  $\psi_{n,0}$  from eq.(8 <sub>$n,0$</sub> ). For each  $\psi_{n,k}$ , the order is: first solve the asymptotic coefficients, from  $s = \frac{1}{2}$  to  $s = L_i - \frac{1}{2}$ ; then solve the Taylor coefficients, from  $a+b = L_f + L_s$  to  $a+b = 0$ (i.e.,  $a = b = 0$ ).

Case 2:  $n$  is an integer. In this case, the order is more complicated, because the operator  $L_n$  has zero eigenvalue(s) in this case. The order is as following:

Step 1: set the asymptotic coefficients and the  $a + b > n$  Taylor coefficients of  $\psi_{n,n}$  to zero;

step 2:  $k \leftarrow n - 1$ ;

step 3: if  $k < 0$ , goto step 8;

step 4: solve the asymptotic coefficients and  $a + b > n$  Taylor coefficients of  $\psi_{n,k}$ , from eq.(8 <sub>$n,k$</sub> ),  
in the order analogous to that of case 1.

step 5: solve the  $a + b = n$  Taylor coefficients of  $\psi_{n,k+1}$ , from eq.(8 <sub>$n,k$</sub> ).

step 6: solve the  $a + b < n$  Taylor coefficients of  $\psi_{n,k+1}$ , from eq.(8 <sub>$n,k+1$</sub> ), with  $a + b$  decreasing(analogous to case 1) to 0.

step 7:  $k \leftarrow k - 1$ , and goto step 3;

step 8: set the  $a + b = n$  Taylor coefficients of  $\psi_{n,0}$  with some free parameters;

step 9: solve the  $a + b < n$  Taylor coefficients of  $\psi_{n,0}$ , from eq.(8 <sub>$n,0$</sub> ), with  $a + b$  decreasing(analogous to case 1) to 0.

The free parameters in solving eq.(8)(see step 8 of case 2) are finally determined by the boundary condition:  $\psi \rightarrow 0$ , when  $t \rightarrow +\infty$ . In principle, we can use the Bartlett-Fock expansion (eq.(4)) for arbitrary  $t$ , because it is always convergent. But actually, when  $t$  is large, the convergency is slow and there is canceling of large numbers before this convergency is reached, both of which make the Bartlett-Fock expansion impractical. So I only use this expansion when  $t$  is relatively small(see ref.[15] for similarity):  $\sqrt{t} \leq \rho_0$ .

In atual calculation, I chose  $L_f = 100$ ,  $L_s = 20$ ,  $L_i = 6$ ,  $n_{max} = 7.5$  (the largest  $n$  value of the terms in eq.(4) that are not neglected), and  $\rho_0 = 0.4$ , and found that the numerical error for the calculation of the inner region ( $\sqrt{t} \leq \rho_0$ ) wavefunction is no more than a few parts in  $10^{10}$ . I use this method to test the accuracy of the calculation: set  $E$  in eq.(8) (note that  $p \equiv -E/2$ ) equal to an initial value (for example, set  $E_{initial} = -2.9037$ , or set  $E_{initial} = -2.903724377$ ), and use the approximate wavefunction  $\psi_{app}$  thus obtained to calculate the value  $(H\psi_{app})/\psi_{app}$ , where  $H$  is the exact Hamiltonian operator, and I find it to be almost equal to the initial value  $E_{initial}$ , with a relative error no more than a few parts in  $10^{10}$ .

When  $t$  is larger, another approach is used:

### 3 THE HYPER-ANGULAR DEPENDENCE OF THE WAVEFUNCTION

We have seen that the hyper-angular dependence of the wavefunction, described as a function of  $(\alpha, \beta)$  for each fixed  $\rho \equiv \sqrt{t} \equiv \sqrt{r_1^2 + r_2^2}$ , has singularities at  $\alpha = \pm 1$  and at  $\beta = 1$ . Physically, this corresponds to the case that the distance between two of the three particles equals zero. It can be proved that, for a spin-singlet, the following coordinate transformation will eliminate these singularities *thoroughly*:

$$u = \sqrt{\frac{1+\alpha}{2}} + \sqrt{\frac{1-\alpha}{2}} - 1, \quad w = \sqrt{1-\beta}. \quad (12)$$

Equivalently,

$$u = \frac{r_1 + r_2}{\rho} - 1, \quad w = \frac{r_{12}}{\rho}. \quad (13)$$

If the energy-eigenstate  $\psi$  is symmetric under the exchange of  $r_1$  and  $r_2$  (spin-singlet), I believe that, for each fixed  $\rho$ ,  $\psi$  is a *entire* function of  $(u, w)$ . If the energy-eigenstate  $\psi$  is antisymmetric under the interchange of  $r_1$  and  $r_2$  (spin-triplet), I believe that, for each fixed  $\rho$ ,  $\psi = \frac{r_1 - r_2}{\rho} \phi$ , where  $\phi$  is a *entire* function of  $(u, w)$ .

This beautiful characteristic makes it especially appropriate to approximate  $\psi$ , for each fixed  $\rho$ , by an  $n$ -order polynomial of  $(u, w)$ , not by an  $n$ -order polynomial of  $(\alpha, \beta)$ . The former expansion, a polynomial of  $(u, w)$ , matches the analytical structure of  $\psi$ ; while the latter one, a polynomial of  $(\alpha, \beta)$ , does not. The hyper-spherical harmonic function method belongs to the latter expansion, a polynomial of  $(\alpha, \beta)$ . So the hyper-spherical harmonic function expansion does not correctly reflect the analytical structure of  $\psi$ . The slow convergency of the hyper-spherical harmonic function expansion is only a consequence of this analytical structure mismatching.

We expect that the  $(u, w)$  polynomial expansion converges *factorially* to the true wavefunction. It is worthful to demonstrate a similar example to illustrate this. Consider a function  $f(x) = \exp(-x)$ ,  $-1 \leq x \leq +1$ ; expand  $f(x)$  by Legendre polynomials:  $f(x) \doteq \sum_{l=0}^n f_l P_l(x)$ ; it can be proved that the error of this formula is of the order  $1/(2^n n!)$ , which factorially approach zero as  $n$  increases.

Using the  $(\rho, u, w)$  coordinates, one can write the Schrödinger equation as:

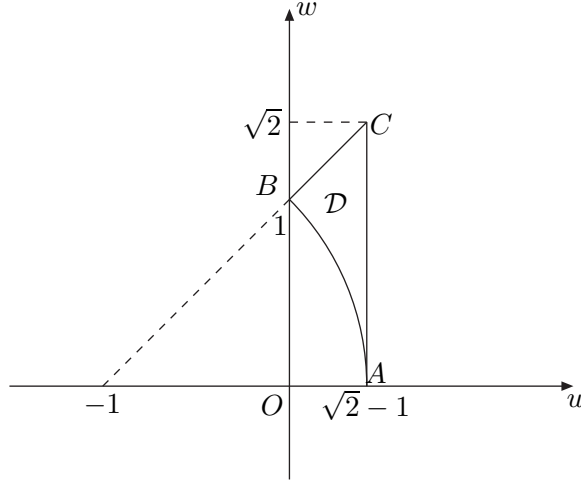
$$-\frac{1}{2}(\partial_\rho^2 + \frac{5}{\rho}\partial_\rho + \frac{4L_0}{\rho^2})\psi + \frac{C}{\rho}\psi = E\psi, \quad (14)$$

where  $L_0$  and  $C$  are the hyper-angular parts of the kinetic energy and the potential energy, respectively.

$$4L_0 = (1-2u-u^2)\partial_u^2 + (2-w^2)\partial_w^2 - \frac{2(1+u)(1-2u-u^2)}{u(2+u)}\frac{(1-w^2)}{w}\partial_u\partial_w + \frac{(1+u)(4-10u-5u^2)}{u(2+u)}\partial_u + \frac{4-5w^2}{w}\partial_w; \quad (15)$$

$$C = -\frac{4(1+u)}{u(2+u)} + \frac{1}{w}. \quad (16)$$

The physical area  $\mathcal{D}$  of  $(u, w)$  is:



In this figure, point  $A$  corresponds to the coincidence of the two electrons, and point  $B$  corresponds to the coincidence of the nucleus and one electron.

For a spin-singlet, we can use an  $n$ -order polynomial of  $(u, w)$  to approximate  $\psi$ . The coefficients of this polynomial are functions of  $\rho$ . Denote by  $\mathcal{L}_N$  the set of all the polynomials of  $(u, w)$  with order no more than  $n$ . Here,  $N = (n+1)(n+2)/2$  is the dimension. In the physical area  $\mathcal{D}$ , I choose a set of points as sample points:

$$w_a = \sqrt{2} \frac{(a_2 + 0.5)}{n_2}, \quad (17)$$

$$u_a = (\sqrt{2} - 1) - [(\sqrt{2} - 1) - m(w_a)] \frac{(a_1 + 0.5)}{n_1}, \quad (18)$$

where  $m(w)$  is the minimum physical  $u$  value for a  $w$  value.  $m(w) = \sqrt{2 - w^2} - 1$ , if  $w < 1$ ; and  $m(w) = w - 1$ , if  $w \geq 1$ .  $a \equiv (a_1, a_2)$ , and  $0 \leq a_1 < n_1$ ,  $0 \leq a_2 < n_2$ . I chose  $n_1 = n_2 = 2n$ , so there are altogether  $4n^2$  sample points. These sample points define a pseudo-innerproduct. I constructed a set of pseudo-orthonormal basis in  $\mathcal{L}_N$ , by using the Schmidt orthogonalization method, and then reduce the operators  $L_0$  and  $C$  to  $N \times N$  matrices under this basis, using the method introduced in section 1.

## 4 CONNECTION OF THE INNER REGION AND THE OUTER REGION WAVEFUNCTIONS

In the area  $\rho < \rho_0$  (inner region), the Bartlett-Fock expansion is used. In the area  $\rho > \rho_0/2$  (outer region),  $\psi$  is approximated by a vector in  $\mathcal{L}_N$  for each given  $\rho$ , and the partial derivatives with respect to  $\rho$  are substituted by optimized variable-order and variable-step differences, which requires the selection of a discrete set of  $\rho$  values. The overlap region of the inner region and the outer region ensures the natural connection of the derivative of  $\psi$ , as well as the connection of  $\psi$  itself. The connection is performed by using the least square method: for a polynomial of  $(u, w)$  at  $\rho = \rho_0$ , appropriately choose the values of the free parameters of the solution of eq.(8) (see section 2) so

that the sum of the squares of the differences of the the inner region solution and the outer region polynomial at the sample points is minimized. This defines a linear transformation to calculate the values of those free parameters from the given polynomial. When the values of these free parameters are determined, one can calculate the values of  $\psi$  in the region  $\rho_0/2 < \rho < \rho_0$ , using the Bartlett-Fock solution, and further use these  $\psi$  values to construct polynomials of  $(u, w)$  at  $\rho_0/2 < \rho < \rho_0$  (according to the law of least square), and then use these polynomials in the difference calculation of the partial derivative of  $\psi$  with respect to  $\rho$  at  $\rho \geq \rho_0$ . At a sufficient large value  $\rho = \rho_1$ , the first-class boundary condition is exerted; of course, future development may substitute this by a connection with the long range asymptotic solution of  $\psi$ .

At last, the whole Schrödinger equation is reduced to an eigen-problem of a finite-dimensional matrix. The dimension of the matrix is  $N_\rho \times N$ , where  $N_\rho$  is the number of free  $\rho$  nodes used in discretizing the partial derivatives with respect to  $\rho$ , and  $N$  is the number of independent hyper-angular polynomials used. Note that the energy value should be used in solving eq.(8), but it is unknown. The actual calculation is thus an iteration process: choose an initial value of  $E_0$  to solve eq.(8) and form the  $N_\rho \times N$  dimensional matrix, and calculate the eigenvalue of this matrix to get a new value  $E_1$ , etc.. The final result is the fixed point of this iteration process. In actual calculation, I found that the convergency of this iteration process is very rapid if  $\rho_0$  is relatively small. Choosing  $\rho_0 = 0.4$ , I found that each step of iteration cause the difference between the eigenvalue of the matrix and the fixed point decrease by about  $(-160)$  times, when calculating the ground state.

## 5 NUMERICAL RESULT AND COMPARISONS

Using 20 independent Bartlett-Fock series(up to the  $t^{7.5}$  term in eq.(4), neglecting higher order terms), choosing  $n = 10$  (so that  $N = 66$ ), choosing  $N_\rho = 40$ , with  $\rho_0 = 0.4$  and  $\rho_1 \doteq 11.32$ , and with the discrete values of  $\rho$  equal to  $0.4/1.2^3, 0.4/1.2^2, 0.4/1.2, 0.4, 0.4 \times 1.2, 0.4 \times 1.2^2, 0.4 \times 1.2^3, \dots, 0.4 \times 1.2^8 \doteq 1.7199, 0.4 \times 1.2^8 + 0.3, 0.4 \times 1.2^8 + 0.6, 0.4 \times 1.2^8 + 0.9, \dots, 0.4 \times 1.2^8 + 9.3$ , and  $0.4 \times 1.2^8 + 9.6 \doteq 11.32$  (the first three points are for the natural connection of the derivative of  $\psi$ , the last point is for the first-class boundary condition, and the remained 40 points are free nodes), and discretizing the partial derivatives with respect to  $\rho$  according to the complex-plane-division rule(that is: when calculating the partial derivatives with respect to  $\rho$  at  $\rho = l$ , use and only use those node points satisfying  $\rho > l/2$  in the difference format, because the point  $\rho = 0$  is the singular point), I obtained the result for the ground state energy of the ideal helium atom:

$$E = -2.9037243738 \ , \quad (19)$$

compared with the accurate value:

$$E = -2.9037243770 \ . \quad (20)$$

So the relative error of the result (19) is about  $1.1 \times 10^{-9}$ . Since my method is not a variational method, the error of the approximate wavefunction that I obtained should be of a similar order of magnitude, so if one calculate the expectation value of the Hamiltonian under this approximate wavefunction, the accuracy of the energy will be further raised by several orders of magnitude.

The result (19) is much more accurate than the result of ref.[10]:  $-2.90359$ , which used the hyper-spherical coordinate method. In ref.[10], the quantum numbers  $(l_1, l_2)$  (angular momenta of the two electrons) are used and a cutoff for them is made; this cutoff does not correctly reflect the analytical structure of  $\psi$  at  $r_{12} = 0$  (equivalently  $\beta = 1$ ). This is the major reason causing the inaccuracy of the result of ref.[10].

It is also worthful to compare my result with that of ref.[4], in which the correlation function hyper-spherical harmonic method is used. Note that the result (19) is obtained by using a set of  $N = 66$  hyper-radius-dependent coefficients to expand the wavefunction. For a similar size in ref.[4],  $N=64$ , the result is  $-2.903724300$ , with relative error about  $26.5 \times 10^{-9}$ . When  $N=169$ , the result of ref.[4] is  $-2.903724368$ , with relative error about  $3.1 \times 10^{-9}$ . Apparently my method converges more rapidly than that of ref.[4]. The major reason is that the correlation function hyper-spherical harmonic method does not cancel the singularities totally—there is still some discontinuity for the higher order derivatives, although the low order singularities, which trouble the naive hyperspherical harmonic method, are canceled by the correlation function.

## 6 CONCLUSIONS, DISCUSSIONS AND FUTURE DEVELOPMENTS

In conclusion, there are several important ideas in my work that should be emphasized: first, I use the asymptotic series to compute the Bartlett-Fock series up to a high precision, with error no more than, for example, a few parts in  $10^{10}$ . Second, I propose an alternative coordinate system, the  $(u, w)$  system, in which the hyper-angular singularities are thoroughly eliminated, which renders a factorial convergency for the expansion of the hyper-angular function. Third, I make use of the least square method to reduce an operator(infinite dimensional matrix) to a finite dimensional matrix in a finite dimensional subspace of the Hilbert space and to connect the solutions in different regions, avoiding complicated numerical integrations, without much loss of the accuracy for the solution. Fourth, the optimized difference format —the complex plane division rule—is used to discretize the partial derivatives of the wavefunction with respect to  $\rho$ . I calculated the ground state energy of an ideal helium atom concretely and obtained a very high precision, demonstrating that my method is superior to many other methods and competitive with any sophisticated methods.

About the analytical structure of the stationary wavefunction: 1. there are logarithmic singularities at  $\rho = 0$ , in the forms of  $\rho^m(\ln \rho)^k$ ; 2. for a given  $\rho$ ,  $\psi$  (for a spin-singlet) or  $\psi/[(r_1 - r_2)/\rho]$ (for a spin-triplet) has no singularity, as a function of  $(u, w)$ .

Here, I must mention the well known variational method based on the Hyleraas-type functions, because it also satisfies the second characteristic of the wavefunction mentioned in the above paragraph. One can see this by a simple derivation. The Hyleraas-type function is a entire function of  $r_1$ ,  $r_2$  and  $r_{12}$ , or equivalently, a entire function of  $r_1 + r_2$ ,  $r_1 - r_2$ , and  $r_{12}$ . For a fixed  $\rho$ , one can substitute  $(r_1 - r_2)^2$  in this function by  $2\rho^2 - (r_1 + r_2)^2$ , so that, for fixed  $\rho$ , the function is a entire function of  $r_1 + r_2$  and  $r_{12}$  for spin-singlet, or such kind of entire function times a common factor  $r_1 - r_2$  for spin-triplet. Equivalently, for fixed  $\rho$ , the Hyleraas-type function is a entire function of  $(u, w)$ (spin-singlet) or such kind of entire function times  $\frac{r_1 - r_2}{\rho}$ (spin-triplet). This characteristic is one of the most important reasons that account for the high accuracy of the Hyleraas-type variational method.

But this variational method also has its shortcoming: the Hyleraas-type function does not reflect the logarithmic singularities with respect to  $\rho$ . So, although this method has high precision for the energy levels, the approximate wavefunctions that it renders may deviate significantly from the true wavefunctions near the origin. See ref.[4,13,14] for detailed discussions.

A central idea of this paper is: devising the calculation method according to the analytical structure of the true solution. The  $(u, w)$  coordinates, the Bartlett-Fock expansion and the asymptotic series approach to compute this expansion, and the complex-plane-division rule in calculating the partial derivatives with respect to  $\rho$ , all reflect this central idea. The basic principle that ensures high numerical precision is just this idea.

This preliminary work is incomplete in the following aspects:

First, how to *prove* that  $\psi$ (for spin-singlet, or  $\psi/[(r_1 - r_2)/\rho]$  for spin-triplet) has no singularity for fixed  $\rho$ , as a function of  $(u, w)$ ? Note that if this function still has singularities outside of the physical area  $\mathcal{D}$ (see previous figure), the convergency of the expansion of the hyper-angular function will be only exponential, not factorial. Of course, even if such kind of singularities do exist, my method will still converge more rapidly than the correlation function hyperspherical harmonic method, because the latter method only converges like  $N^{-p}$ , slower than  $\exp(-\gamma\sqrt{N})$ . The rapid convergency of my method make me guess that such kind of singularities do not exist.

Second, the asymptotic behavior of the wavefunction, when one electron is far away from the nucleus, is not studied in this work. This problem will be important when the highly excited states and the scattering states are studied, a topic that will become my next object.

Third, how to use the ideas proposed in this work to study a helium atom with finite nuclear mass? Besides this, the relativistic and QED corrections must be calculated, if one want to obtain a result comparable with high-precision experiments.

Fourth, I have focused on the S states till now. When the total angular momentum is not zero, there might be more than one distance-dependent functions (see, for example, ref.[11]). I believe that some important analytical structures of the S states studied in this work are also valid for those functions.

Surely, some important aspects of this work will also play an important role in the highly excited states and the scattering states: the logarithmic singularities about  $\rho$  and the method to compute the Bartlett-Fock expansion, the non-singularity with respect to the coordinates  $(u, w)$ , and the technique to connect solutions of different regions, etc.. They can be applied to the study of the highly excited states and the scattering states.

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